

Author Index to Volume 151

- Al-Adel, F.F., see P.J. Jewsbury 151 (1991) 103
- Albinsson, B., S. Eriksson, R. Lyng and M. Kubista, The electronically excited states of 2-phenylindole 151 (1991) 149
- Alcamí, M., O. Mó and M. Yáñez, Ab initio molecular orbital treatment of hydroxylamine- X^+ -water and hydroxylamine- X^+ -ammonia ($X=H, Li$) clusters 151 (1991) 21
- Andrés, J.L., M. Duran, A. Lledós and J. Bertrán, Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide 151 (1991) 37
- Bakowies, D. and W. Thiel, Theoretical infrared spectra of large carbon clusters 151 (1991) 309
- Bates Jr., R.D., see K.L. McNesby 151 (1991) 385
- Bates Jr., R.D., see K.L. McNesby 151 (1991) 401
- Baumgärtel, H., see R. Loch 151 (1991) 137
- Bauschlicher Jr., C.W., see M. Rosi 151 (1991) 1
- Beddard, G.S., see M.G. Hyde 151 (1991) 239
- Bencivenni, L., see F. Ramondo 151 (1991) 179
- Bertrán, J., see J.L. Andrés 151 (1991) 37
- Bondybey, V.E., see I. Fischer 151 (1991) 295
- Bonomo, R.P., A.J. Di Bilio and F. Riggi, EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra 151 (1991) 323
- Brion, C.E., see W. Zhang 151 (1991) 343
- Brion, C.E., see W. Zhang 151 (1991) 357
- Brunner, H., see R.H. Fritsch 151 (1991) 261
- Burri, J. and H. Fischer, Degenerate triplet spin exchange in liquid solution studied by pulse NMR 151 (1991) 279
- Burris, J., J. Butler, T. McGee and W. Heaps, Quenching and rotational transfer rates in the $v'=0$ manifold of $OH(A^2\Sigma^+)$ 151 (1991) 233
- Butler, J., see J. Burris 151 (1991) 233
- Caminiti, R., see F. Ramondo 151 (1991) 179
- Castellucci, E., see A. Tafi 151 (1991) 205
- Čejchan, A., see V. Špirko 151 (1991) 45
- Chaumet, M., see K. Rościszewski 151 (1991) 159
- Cooper, G., see W. Zhang 151 (1991) 343
- Cooper, G., see W. Zhang 151 (1991) 357
- Deakyne, C.A., see M. Shen 151 (1991) 187
- Di Bilio, A.J., see R.P. Bonomo 151 (1991) 323
- Dierksen, G.H.F., see V. Špirko 151 (1991) 45
- Domcke, W., see M. Seel 151 (1991) 59
- Donovan, R.J., see P.J. Jewsbury 151 (1991) 103
- Duran, M., see J.L. Andrés 151 (1991) 37

- Düren, R., R.K.B. Helbing and S. Milošević, Model study of the effect of anisotropy on the differential cross section for atom-molecule scattering: the double rainbows 151 (1991) 287
- Eriksson, S., see B. Albinsson 151 (1991) 149
- Fischer, H., see J. Burri 151 (1991) 279
- Fischer, I., V.E. Bondybey, P. Rosmus and H.-J. Werner, Theoretical study of the electronic states of BeLi and Be₂⁺ 151 (1991) 295
- Fritsch, R.H., H. Brunner and K.H. Hausser, Triplet electron-proton cross-polarization by satisfying a modified Hartmann-Hahn condition 151 (1991) 261
- Fulde, P., see K. Rościszewski 151 (1991) 159
- Gale, G.M. and P. Schanne, Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal 151 (1991) 127
- García de la Vega, J.M. and E. San Fabián, Jahn-Teller effect and dissociation from the ground state of CF₄⁺ 151 (1991) 335
- Hagenow, G., see R. Loch 151 (1991) 137
- Hausser, K.H., see R.H. Fritsch 151 (1991) 261
- Heaps, W., see J. Burris 151 (1991) 233
- Heaven, M.C., see M. Macler 151 (1991) 219
- Helbing, R.K.B., see R. Düren 151 (1991) 287
- Herman, Z., see J. Vančura 151 (1991) 249
- Hottmann, K., see R. Loch 151 (1991) 137
- Hougen, J.T., see P. Uijt de Haag 151 (1991) 371
- Hyde, M.G. and G.S. Beddard, Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine 151 (1991) 239
- Ibuki, T., see W. Zhang 151 (1991) 343
- Ibuki, T., see W. Zhang 151 (1991) 357
- Jewsbury, P.J., K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan, Determination of the radiative lifetimes of nine ion-pair states of I₂ 151 (1991) 103
- Juzeliūnas, G., Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains 151 (1991) 169
- Kashiwagi, H., see Y. Mochizuki 151 (1991) 11
- Kubista, M., see B. Albinsson 151 (1991) 149
- Kuntz, P.J., B.I. Niefer and J.J. Sloan, A multisurface classical trajectory study of the dynamics of the reaction O(¹D₂) + H₂ → OH(*v'*, *J'*, *θ'*) + H using the diatomics in molecules method 151 (1991) 77
- Langhoff, S.R., see M. Rosi 151 (1991) 1
- Langridge-Smith, P.R.R., see P.J. Jewsbury 151 (1991) 103
- Lawley, K.P., see P.J. Jewsbury 151 (1991) 103
- Lipkin, N., see N. Rom 151 (1991) 199
- Lledós, A., see J.L. Andrés 151 (1991) 37

- Lobo, R.F.M. and A.M.C. Moutinho, A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation 151 (1991) 95
- Locht, R., G. Hagenow, K. Hottmann and H. Baumgärtel, Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O 151 (1991) 137
- Lyng, R., see B. Albinsson 151 (1991) 149
- Macler, M. and M.C. Heaven, Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices 151 (1991) 219
- McGee, T., see J. Burris 151 (1991) 233
- McNesby, K.L. and R.D. Bates Jr., Secondary heating effects in laser-induced fluorescence experiments 151 (1991) 385
- McNesby, K.L. and R.D. Bates Jr., CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O 151 (1991) 401
- Meerts, W.L., see P. Uijt de Haag 151 (1991) 371
- Meerts, W.L., see E. Zwart 151 (1991) 407
- Milošević, S., see R. Dören 151 (1991) 287
- Mó, O., see M. Alcamí 151 (1991) 21
- Mochizuki, Y., K. Tanaka and H. Kashiwagi, Electronic structure of linear form of OCuO 151 (1991) 11
- Moiseyev, N., see N. Rom 151 (1991) 199
- Momicchioli, F., see G. Ponterini 151 (1991) 111
- Moutinho, A.M.C., see R.F.M. Lobo 151 (1991) 95
- Niefer, B.I., see P.J. Kuntz 151 (1991) 77
- Pawlikowski, M. and O. Sonnich Mortensen, Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes 151 (1991) 73
- Ponterini, G. and F. Momicchioli, Trans-cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models 151 (1991) 111
- Procacci, P., see A. Tafi 151 (1991) 205
- Ramondo, F., L. Bencivenni, R. Caminiti and C. Sadun, Ab initio SCF study on LiClO_4 and Li_2SO_4 molecules: geometries and vibrational frequencies 151 (1991) 179
- Ridley, T., see P.J. Jewsbury 151 (1991) 103
- Riggi, F., see R.P. Bonomo 151 (1991) 323
- Rom, N., N. Lipkin and N. Moiseyev, Optical potentials by the complex coordinate method 151 (1991) 199
- Rościszewski, K., M. Chaumet and P. Fulde, Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms 151 (1991) 159
- Rosi, M., C.W. Bauschlicher Jr. and S.R. Langhoff, Theoretical study of the spectroscopy of Al_2^+ 151 (1991) 1
- Rosmus, P., see I. Fischer 151 (1991) 295
- Sadun, C., see F. Ramondo 151 (1991) 179
- Salvi, P.R., see A. Tafi 151 (1991) 205
- San Fabián, E., see J.M. García de la Vega 151 (1991) 335
- Schaefer III, H.F., see M. Shen 151 (1991) 187

- Schanne, P., see G.M. Gale 151 (1991) 127
- Seel, M. and W. Domcke, Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling 151 (1991) 59
- Shen, M., Y. Xie, H.F. Schaefer III and C.A. Deakyne, The $\text{H}_2\text{O}_2\text{-NO}_2^-$ and H_2NO_4^- isomers of the nitrate anion-water complex 151 (1991) 187
- Sloan, J.J., see P.J. Kuntz 151 (1991) 77
- Sonnich Mortensen, O., see M. Pawlikowski 151 (1991) 73
- Špirko, V., A. Čejchan and G.H.F. Dierksen, Rotation-vibration energies of FHF^- and ClHCl^- from high-level correlated calculations of potential energy surfaces 151 (1991) 45
- Tafi, A., P. Procacci, E. Castellucci and P.R. Salvi, Polar phonons in SO_2 single crystal 151 (1991) 205
- Tanaka, K., see Y. Mochizuki 151 (1991) 11
- Thiel, W., see D. Bakowies 151 (1991) 309
- Uijt de Haag, P., W.L. Meerts and J.T. Hougen, A study of the S_1 $6^1(^1\text{A}_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy 151 (1991) 371
- Vančura, J. and Z. Herman, Hydroxonium ion formation in collisions of $\text{H}_2\text{O}^+ + \text{D}_2\text{O}$ and $\text{D}_2\text{O}^+ + \text{H}_2\text{O}$: a crossed-beam scattering study 151 (1991) 249
- Werner, H.-J., see I. Fischer 151 (1991) 295
- Xie, Y., see M. Shen 151 (1991) 187
- Yáñez, M., see M. Alcamí 151 (1991) 21
- Zhang, W., G. Cooper, T. Ibuki and C.E. Brion, Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl 151 (1991) 343
- Zhang, W., G. Cooper, T. Ibuki and C.E. Brion, Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 151 (1991) 357
- Zwart, E. and W.L. Meerts, The submillimeter rotation-tunneling spectrum of $\text{Ar-D}_2\text{O}$ and Ar-NH_3 151 (1991) 407

List of Subjects

1 Methods

1.1 Theoretical

- 1.1.1 Group theory and algebras
- 1.1.2 Classical mechanics *
- 1.1.3 Quantized field theory
- 1.1.4 Many body and quasiparticle approaches *
- 1.1.5 Coupling schemes and perturbative treatments
- 1.1.6 Relativistic quantum mechanics
- 1.1.7 Transport quantum mechanics
- 1.1.8 Equilibrium statistical mechanics
- 1.1.9 Statistical mechanics of stationary states
- 1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories
- 1.1.11 Ab initio schemes for stationary properties *
- 1.1.12 Computational and simulation methods *
- 1.1.13 Molecular dynamics and scattering theory *

1.2 Experimental

- 1.2.1 Magnetic resonances *
- 1.2.2 Cyclotron resonance
- 1.2.3 Microwave spectroscopy *
- 1.2.4 Infrared spectroscopy *
- 1.2.5 Raman spectroscopy *
- 1.2.6 Visible and UV spectroscopy *
- 1.2.7 Fluorescence spectroscopy *
- 1.2.8 Photoelectron and Auger spectroscopy
- 1.2.9 X-ray spectroscopy
- 1.2.10 Electron impact spectroscopy *
- 1.2.11 Laser methods *
- 1.2.12 Picosecond spectroscopy *
- 1.2.13 Non-linear optical spectroscopy *
- 1.2.14 Synchrotron spectroscopies *
- 1.2.15 Coherent optical spectroscopy
- 1.2.16 Optical pumping
- 1.2.17 Multiple resonance spectroscopy *
- 1.2.18 Optoacoustic spectroscopy
- 1.2.19 Atomic and molecular beam techniques *
- 1.2.20 Time-resolved experiments *
- 1.2.21 Mass spectrometry *
- 1.2.22 Radiolysis
- 1.2.23 Mössbauer spectroscopy
- 1.2.24 X-ray, electron and neutron diffraction
- 1.2.25 Neutron scattering
- 1.2.26 Light scattering
- 1.2.27 Field emission and field ionization
- 1.2.28 Measurement of macroscopic variables

2 Objects

2.1 Bulk systems

- 2.1.1 Gases
- 2.1.2 Supersonic beams
- 2.1.3 Liquids neat
- 2.1.4 Liquid mixtures and solutions *
- 2.1.5 Crystals *
- 2.1.5.1 neat *
- 2.1.5.2 mixed *
- 2.1.6 Glasses
- 2.1.7 Liquid crystals
- 2.1.8 Polymers
- 2.1.9 Semiconductors
- 2.1.10 Metals and alloys *
- 2.1.11 Thin films
- 2.1.12 Surfaces
- 2.1.13 Low-dimensional materials
- 2.1.14 Dielectrics
- 2.1.15 Plasmas
- 2.1.16 Biological systems

2.2 Microscopic systems

- 2.2.1 Atoms
- 2.2.2 Molecules (neutral and ionic) *
- 2.2.2.1 diatomic *
- 2.2.2.2 small polyatomics *
- 2.2.2.3 aromatics *
- 2.2.2.4 other large *
- 2.2.2.5 polymeric and biological
- 2.2.3 Molecular aggregates *
- 2.2.3.1 dimers
- 2.2.3.2 van der Waals molecules *
- 2.2.3.3 clusters *
- 2.2.3.4 complexes *
- 2.2.4 Free radicals (including hydronium and muonium)
- 2.2.5 Quasiparticles (including excitons) *
- 2.2.6 Defects and impurities
- 2.2.7 Ions and charge carriers *

* Denotes subjects covered in this volume

3 Phenomena

- 3.1 Molecular structure *
- 3.2 Vibrations and rotations of molecules *
- 3.3 Electronic structure and states *
- 3.4 Electric and magnetic properties *
- 3.5 Spin splittings *
- 3.6 Optical activity *
- 3.7 Molecular interactions *
- 3.8 Spectral bandshapes and intensities *
- 3.9 Coupling of electronic and nuclear motion *
- 3.10 Energy transfer processes *
- 3.11 Molecular photophysical processes *
- 3.12 Intramolecular dynamics *
 - 3.12.1 radiationless transitions *
 - 3.12.2 vibrational energy redistribution (including vibrational dissociation)
- 3.13 Luminescence spectra, yields and lifetimes *
- 3.14 Coherence loss processes *
- 3.15 Non-linear responses (including optical)
- 3.16 Multiphoton phenomena
- 3.17 Reactions (including dissociation) *
 - 3.17.1 gas phase *
 - 3.17.2 condensed phase
 - 3.17.3 photochemical *
- 3.18 Tunnelling *
- 3.19 Electron transfer *
- 3.20 Positron annihilation
- 3.21 Ionization (including Rydberg states) *
- 3.22 Molecular motion (including diffusive) *
- 3.23 Isotopic effects
- 3.24 Fluctuations and noise
- 3.25 Collective motion and excitations
- 3.26 Surface effects and catalysis
- 3.27 Thermodynamic and transport properties
- 3.28 Structure of solids and liquids
- 3.29 Critical phenomena
- 3.30 Phase transitions

Subject Index to Volume 151

Methods

Theoretical

Classical mechanics

- A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2) + H_2 \rightarrow OH(v', J', \theta') + H$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77

Many body and quasiparticle approaches

- Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms, K. Rościszewski, M. Chaumet and P. Fulde 151 (1991) 159
- Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169

Ab initio schemes for stationary properties

- Theoretical study of the spectroscopy of Al_2^+ , M. Rosi, C.W. Bauschlicher Jr. and S.R. Langhoff 151 (1991) 1
- Electronic structure of linear form of $OCuO$, Y. Mochizuki, K. Tanaka and H. Kashiwagi 151 (1991) 11
- Ab initio molecular orbital treatment of hydroxylamine- X^+ -water and hydroxylamine- X^+ -ammonia ($X=H, Li$) clusters, M. Alcamí, O. Mó and M. Yáñez 151 (1991) 21
- Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
- Rotation-vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Dierksen 151 (1991) 45
- Ab initio SCF study on $LiClO_4$ and Li_2SO_4 molecules: geometries and vibrational frequencies, F. Ramondo, L. Bencivenni, R. Caminiti and C. Sadun 151 (1991) 179
- The $H_2O_2-NO_2^-$ and $H_2NO_4^-$ isomers of the nitrate anion-water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
- Theoretical study of the electronic states of $BeLi$ and Be_2^+ , I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295
- Jahn-Teller effect and dissociation from the ground state of CF_4^+ , J.M. García de la Vega and E. San Fabián 151 (1991) 335

Computational and simulation methods

- Rotation-vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Dierksen 151 (1991) 45
- Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling, M. Seel and W. Domcke 151 (1991) 59
- Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199

- Polar phonons in SO₂ single crystal, A. Tafi, P. Procacci, E. Castellucci and P.R. Salvi 151 (1991) 205
Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323

Molecular dynamics and scattering theory

- Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
A multisurface classical trajectory study of the dynamics of the reaction O(¹D₂) + H₂ → OH(*v'*, *J'*, *θ'*) + H using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77
A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95
Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
Model study of the effect of anisotropy on the differential cross section for atom-molecule scattering: the double rainbows, R. Dören, R.K.B. Helbing and S. Milošević 151 (1991) 287

Experimental

Magnetic resonances

- Triplet electron-proton cross-polarization by satisfying a modified Hartmann-Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323

Microwave spectroscopy

- The submillimeter rotation-tunneling spectrum of Ar-D₂O and Ar-NH₃, E. Zwart and W.L. Meerts 151 (1991) 407

Infrared spectroscopy

- The submillimeter rotation-tunneling spectrum of Ar-D₂O and Ar-NH₃, E. Zwart and W.L. Meerts 151 (1991) 407

Raman spectroscopy

- Polar phonons in SO₂ single crystal, A. Tafi, P. Procacci, E. Castellucci and P.R. Salvi 151 (1991) 205

Visible and UV spectroscopy

- The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
Quenching and rotational transfer rates in the *v'* = 0 manifold of OH(A²Σ⁺), J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233

- Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
- Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
- A study of the S_1 $6^1(^1A_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
- Fluorescence spectroscopy*
- The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
- Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
- Quenching and rotational transfer rates in the $v' = 0$ manifold of $\text{OH}(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
- Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
- Electron impact spectroscopy*
- Jahn–Teller effect and dissociation from the ground state of CF_4^+ , J.M. García de la Vega and E. San Fabián 151 (1991) 335
- Laser methods*
- Determination of the radiative lifetimes of nine ion-pair states of I_2 , P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
- Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
- CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O , K.L. McNesby and R.D. Bates Jr. 151 (1991) 401
- Picosecond spectroscopy*
- Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
- Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
- Non-linear optical spectroscopy*
- Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
- Synchrotron spectroscopies*
- Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O , R. Loch, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137
- Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357

Multiple resonance spectroscopy

- Determination of the radiative lifetimes of nine ion-pair states of I_2 , P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103

Atomic and molecular beam techniques

- A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95
- Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249

Time-resolved experiments

- Determination of the radiative lifetimes of nine ion-pair states of I_2 , P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
- Trans-cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
- Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
- CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O , K.L. McNesby and R.D. Bates Jr. 151 (1991) 401

Mass spectrometry

- A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95
- Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O , R. Locht, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137
- Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249
- Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343

Objects**Bulk systems***Liquid mixtures and solutions*

- Ab initio molecular orbital treatment of hydroxylamine- X^+ -water and hydroxylamine- X^+ -ammonia ($X=H, Li$) clusters, M. Alcamí, O. Mó and M. Yáñez 151 (1991) 21
- Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
- Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239

*Crystals**-neat*

- Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal,
G.M. Gale and P. Schanne 151 (1991) 127
- Polar phonons in SO₂ single crystal, A. Tafi, P. Procacci, E. Castellucci and P.R. Salvi 151 (1991) 205

-mixed

- Triplet electron-proton cross-polarization by satisfying a modified Hartmann-Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261

Metals and alloys

- Theoretical study of the electronic states of BeLi and Be₂⁺, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295

Microscopic systems*Molecules (neutral and ionic)*

- Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
- Ab initio SCF study on LiClO₄ and Li₂SO₄ molecules: geometries and vibrational frequencies, F. Ramondo, L. Bencivenni, R. Caminiti and C. Sadun 151 (1991) 179

-diatomic

- Theoretical study of the spectroscopy of Al₂⁺, M. Rosi, C.W. Bauschlicher Jr. and S.R. Langhoff 151 (1991) 1
- Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
- Determination of the radiative lifetimes of nine ion-pair states of I₂, P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
- Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
- Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
- Quenching and rotational transfer rates in the $v' = 0$ manifold of OH(A²Σ⁺), J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
- Theoretical study of the electronic states of BeLi and Be₂⁺, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295

-small polyatomics

- Electronic structure of linear form of OCuO, Y. Mochizuki, K. Tanaka and H. Kashiwagi 151 (1991) 11
- Rotation-vibration energies of FHF⁻ and ClHCl⁻ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Diercksen 151 (1991) 45
- Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO⁺ and O⁺ from N₂O, R. Loch, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137
- Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms, K. Rościszewski, M. Chaumet and P. Fulde 151 (1991) 159

- The $\text{H}_2\text{O}_2\text{--NO}_2^-$ and H_2NO_4^- isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
- Model study of the effect of anisotropy on the differential cross section for atom–molecule scattering: the double rainbows, R. Dören, R.K.B. Helbing and S. Milošević 151 (1991) 287
- Jahn–Teller effect and dissociation from the ground state of CF_4^+ , J.M. García de la Vega and E. San Fabián 151 (1991) 335
- Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
- Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
- A study of the S_1 6^1 ($^1\text{A}_2''$) vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
- Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
- CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O , K.L. McNesby and R.D. Bates Jr. 151 (1991) 401
- aromatics*
- The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
- Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
- Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
- other large*
- Trans–cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
- Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
- Molecular aggregates*
- Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
- van der Waals molecules*
- The submillimeter rotation-tunneling spectrum of $\text{Ar--D}_2\text{O}$ and Ar--NH_3 , E. Zwart and W.L. Meerts 151 (1991) 407
- clusters*
- Theoretical study of the electronic states of BeLi and Be_2^+ , I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295
- complexes*
- A multisurface classical trajectory study of the dynamics of the reaction $\text{O}(^1\text{D}_2) + \text{H}_2 \rightarrow \text{OH}(v', J', \Theta') + \text{H}$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77

- The $\text{H}_2\text{O}_2\text{-NO}_2^-$ and H_2NO_4^- isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
- EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
- Quasiparticles (including excitons)*
- Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
- Ions and charge carriers*
- The $\text{H}_2\text{O}_2\text{-NO}_2^-$ and H_2NO_4^- isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
- Hydroxonium ion formation in collisions of $\text{H}_2\text{O}^+ + \text{D}_2\text{O}$ and $\text{D}_2\text{O}^+ + \text{H}_2\text{O}$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249

Phenomena

Molecular structure

- Ab initio SCF study on LiClO_4 and Li_2SO_4 molecules: geometries and vibrational frequencies, F. Ramondo, L. Bencivenni, R. Caminiti and C. Sadun 151 (1991) 179
- The $\text{H}_2\text{O}_2\text{-NO}_2^-$ and H_2NO_4^- isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
- Jahn–Teller effect and dissociation from the ground state of CF_4^+ , J.M. García de la Vega and E. San Fabián 151 (1991) 335
- The submillimeter rotation-tunneling spectrum of $\text{Ar-D}_2\text{O}$ and Ar-NH_3 , E. Zwart and W.L. Meerts 151 (1991) 407

Vibrations and rotations of molecules

- Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
- Rotation–vibration energies of FHF^- and ClHCl^- from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Dierksen 151 (1991) 45
- A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95
- Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
- Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309

Electronic structure and states

- Theoretical study of the spectroscopy of Al_2^+ , M. Rosi, C.W. Bauschlicher Jr. and S.R. Langhoff 151 (1991) 1
- Electronic structure of linear form of OCuO , Y. Mochizuki, K. Tanaka and H. Kashiwagi 151 (1991) 11
- Ab initio molecular orbital treatment of hydroxylamine– X^+ –water and hydroxylamine– X^+ –ammonia ($\text{X}=\text{H}, \text{Li}$) clusters, M. Alcamí, O. Mó and M. Yáñez 151 (1991) 21
- The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
- Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms, K. Rościszewski, M. Chaumet and P. Fulde 151 (1991) 159

- Quenching and rotational transfer rates in the $v'=0$ manifold of $\text{OH}(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
- Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
- Theoretical study of the electronic states of BeLi and Be_2^+ , I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295
- Jahn-Teller effect and dissociation from the ground state of CF_4^+ , J.M. García de la Vega and E. San Fabián 151 (1991) 335
- Electric and magnetic properties*
- Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
- Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
- Triplet electron-proton cross-polarization by satisfying a modified Hartmann-Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
- Spin splittings*
- EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
- Optical activity*
- Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
- Molecular interactions*
- A multisurface classical trajectory study of the dynamics of the reaction $\text{O}(^1\text{D}_2) + \text{H}_2 \rightarrow \text{OH}(v', J', \theta') + \text{H}$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77
- Model study of the effect of anisotropy on the differential cross section for atom-molecule scattering: the double rainbows, R. Dören, R.K.B. Helbing and S. Milošević 151 (1991) 287
- The submillimeter rotation-tunneling spectrum of $\text{Ar-D}_2\text{O}$ and Ar-NH_3 , E. Zwart and W.L. Meerts 151 (1991) 407
- Spectral bandshapes and intensities*
- Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
- EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
- Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
- Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357

Coupling of electronic and nuclear motion

- Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling, M. Seel and W. Domcke 151 (1991) 59

Energy transfer processes

- Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
- Quenching and rotational transfer rates in the $v'=0$ manifold of $\text{OH}(\text{A}^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
- Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
- A study of the $\text{S}_1 6^1 ({}^1\text{A}_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
- Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
- CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O , K.L. McNesby and R.D. Bates Jr. 151 (1991) 401

Molecular photophysical processes

- Trans-cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
- Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
- Triplet electron-proton cross-polarization by satisfying a modified Hartmann-Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
- Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
- Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357

Intramolecular dynamics

- A multisurface classical trajectory study of the dynamics of the reaction $\text{O}({}^1\text{D}_2) + \text{H}_2 \rightarrow \text{OH}(v', J', \theta') + \text{H}$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77

-radiationless transitions

- Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
- A study of the $\text{S}_1 6^1 ({}^1\text{A}_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371

Luminescence spectra, yields and lifetimes

- Determination of the radiative lifetimes of nine ion-pair states of I_2 , P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
- Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
- Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219

Coherence loss processes

- Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127

Reactions (including dissociation)

- Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O , R. Loch, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137

-gas phase

- Hydroxonium ion formation in collisions of $\text{H}_2\text{O}^+ + \text{D}_2\text{O}$ and $\text{D}_2\text{O}^+ + \text{H}_2\text{O}$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249

-photochemical

- Trans-cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
- Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279

Tunnelling

- Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199

Electron transfer

- A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95

Ionization (including Rydberg states)

- Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling, M. Seel and W. Domcke 151 (1991) 59
- Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O , R. Loch, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137

Molecular motion (including diffusive)

- Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239

